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Lattice Dynamical Study and Elastic Property of Europium Telluride (EuTe) Crystal

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ABSTRACT

In the present work authors are reporting complete lattice dynamical properties of Europium telluride (EuTe). The present model works on three body rigid ion model & three body rigid shell model (TRIM & TRSM). The short-range overlap repulsion is operative up to the second neighboring ions. An excellent agreement has been obtained between theory and experiment for their all-phonon properties of (EuTe) like phonon dispersion curves, Debye temperature variations, two-phonon IR/Raman spectra, third-fourth order lattice constant, pressure derivative and anharmonic elastic properties.

Keywords: Phonon dispersion curves, Debye temperature variations, Two-phonon IR/Raman spectra, Third-fourth order lattice constant, Pressure derivative, Anharmonic elastic properties.

INTRODUCTION

The electronic structure of Europium telluride (EuTe), which is a family of Europium Chalcogenides crystallize in F.C.C. NaCl structure and are also called rare earth europium chalcogenides. Europium Telluride (EuTe) is a crystal grown product generally immediately available in most volumes. Unlike other rare earth compounds europium chalcogenides generally, show non-mixed valance character. Complete experimental data on phonon dispersion is available for EuTe, which has been reported. by Silberstein *et al.,*[1]. Zeyher and Kress[2] discuss the complete phon0n dispersion curves (PDC), combined density of states (CDS)[3] and Debye temperature variations curve given by[4]. The parameters like elastic & dielectric constants[5,6], the physical-natural properties of the (EuTe) have been attracted and their explication through different conceptual models[7-12], which has also satisfyingly narrated their engrossing properties. It has been establishing the interactions of three body which demonstrate the optical branches and Cauchy discrepancy concurrently to almost all the ionic-semiconducting crystals[13]. The remarkable success achieved from (RIM)[14] and (RSM)[15] represent the lattice properties of alkali halides and worthwhile to explore the adequacies of these model for EuTe. The third-order elastic constants (TOEC), which is related to the energy products of three strain

components, and the lowest order constants to enter the description of non-linear effects like the equation of state and the interaction of phonons. These TOEC is determined from velocity measurements on small amplitude sound waves in statically stressed media. The aim of present report is to test the applicability and utility of second-neighbor three-body rigid shell model (TRSM) and second neighbor three-body rigid ion model (TRIM) with the satisfactory description of phonon dispersion relations and other phonon properties of the EuTe.

Theory

The existing model accordingly consists of the comprehensive shield coulomb, TBI and the short-range overrun repulsion effective up to the next-neighbor for EuTe. The relevant expression for the crystal potential per unit cell can be extrapolate TBFSM, is given as

$$\Phi = \Phi^{C} + \Phi^{R} + \Phi^{TBI} \quad (1)$$

where Φ^{C} is comprehensive Coulomb reciprocity potential. where Φ^{R} is a short-range repulsion & Φ^{TBI} long-range TBI interaction potential by[16]. The secular determinant equation is given by:

$$\left| \underline{D}(\vec{q}) - \omega^{2} \underline{M I} \right| = 0 \quad (2)$$

The dipole's (VWI) efficient next- neighbor is given as:

$$\Phi_{dd}^{VWI}(r) = -S_{V} \left| \frac{C_{++} + C_{--}}{6 r^{6}} \right| = \Phi^{V}(r) \quad (3)$$

By use of Eq. (2) the Eq. for elastic constants can give as:

$$C_{11} = \frac{e^{2}}{4r_{0}^{4}} \left[-5.112 Z_{m}^{2} + A_{12} + \frac{1}{2}(A_{11} + A_{22}) + \frac{1}{2}(B_{11} + B_{22}) + 9.3204\ \xi'^{2} \right] \quad (4)$$

$$C_{12} = \frac{e^{2}}{4r_{0}^{4}} \left[0.226\, Z_{m}^{2} - B_{12} + \frac{1}{4}(A_{11} + A_{22}) - \frac{5}{4}(B_{11} + B_{22}) + 9.3204\ \xi'^{2} \right] \quad (5)$$

$$C_{44} = \frac{e^{2}}{4r_{0}^{4}} \left[2.556 Z_{m}^{2} + B_{12} + \frac{1}{4}(A_{11} + A_{22}) + \frac{3}{4}(B_{11} + B_{22}) \right] \quad (6)$$

Vibrational Properties of EuTe

The term fo is based on overlap integrals of charge (e^{-}) wave functions and expressions for optical vibration frequencies (ω_{L} and ω_{T}) are given as:

$$\left(\mu\omega_{L}^{2}\right)_{q=0} = R_{0}' + \frac{(Z'e)^{2}}{v f_{L}} \cdot \frac{8\pi}{3} \left(Z_{m}^{2} + 6\xi'^{2} \right) \quad (7)$$

$$\left(\mu\omega_{T}^{2}\right)_{q=0} = R_{0}' - \frac{(Z'e)^{2}}{v f_{T}} \cdot \frac{4\pi}{3} Z_{m}^{2} \quad (8)$$

By using Debye's model distribution function for frequency is given by

$$\Theta_{D} = h\nu_{m}/K \quad (9)$$

the density of states of phonon for each polarization is given by

$$g(\omega) = dN/d\omega = N \int_{BZ} \sum_{j} \delta\left[\omega - \omega_{j}(q)\right] dq = (VK^{2}/2\pi^{2}).dK/d\omega \quad (10)$$

and $N = (L/2\pi)^{3} (4\pi K^{3}/3)$ and phonon wave vector q such that $\int g(\omega) d\omega = 1$

Numerical computations

The input data and calculated model parameters from SMTRSM and SNTRIM for EuTe are given in Table 2.

Table 1: Cauchy-Discrepancy (in units 10^{12} dyne/cm^2) for EuTe

Cauchy-Discrepancy Property	Values for EuTe
$C_{112} - C_{166}$	-0.3501831
$C_{123} - C_{456}$	0.2610215
$C_{144} - C_{456}$	0.0870346
$C_{123} - C_{144}$	0.1739869
$C_{1112} - C_{1166}$	2.3062965
$C_{1122} - C_{1266}$	0.1261647
$C_{1122} - C_{4444}$	0.637605
$C_{1123} - C_{1144}$	-0.0232144
$C_{1123} - C_{1456}$	-0.1482605
$C_{1123} - C_{1244}$	-0.4385078
$C_{1123} - C_{4466}$	-0.4158073

Table 2: Input data, model parameters for EuTe in-C_{ij} (in 10^{12} dyn/cm^2), ro(in 10^{-8} cm)

Input data for EuTe		Model parameters for EuTe		
Properties	Values for EuTe	Parameters	TRSM	TRIM
C_{11}	9.36	$r_0 f_0'$	-0.0262	-0.0262
C_{12}	0.67	Z_m^2	0.5965	0.5722
C_{44}	1.63	A	12.702	12.6113
r_o	0.24	B	-0.6950	-0.6667
$\alpha 1$	8.76	d_1	0.4136	----------
α_2	3.292	d_2	0.9680	----------
		Y_1	-0.2382	----------
		Y_2	-3.7420	----------

Table 3: Combined Density States curve for EuTe

Raman Active-(Present study) Frequency In (THz)	Branch	Values (cm^{-1})
42	L0(X)-LA(Δ)	43
74	LO(X)–TA(X)	75
116	LA+TA(X)	118
157	LA(X)+TA(Δ)	158
172	2LA(Δ)	172
189	TO+LA(Δ)	189
206	2TO(Δ)	205
234	2LO(X)	233
257	2LO(Δ)	255
287	2LO(┌)	286

Table 4: TOEC & FOEC (in units 10^{12} dyne/ Cm^2), Pressure derivatives of SOEC and TOEC for EuTe

TOEC and FOEC (in units 10^{12} dyn/Cm^2)		Pressure derivatives of SOEC and TOEC(dimensionless)	
Property	EuTe (Present)	Property	EuTe (Present)
C_{111}	2543.4513	dK'/dP	66.328857
C_{112}	-1.9844249	dS'/dP	36.399633
C_{123}	1.2280826	dC'_{44}/dP	-2.7321557
C_{144}	1.0540957	dC'_{111}/dP	-4263.2546
C_{166}	-1.6342418	dC'_{112}/dP	-3.3262317
C_{456}	0.9670611	dC'_{166}/dP	2.7392656
C_{1111}	3483.4014	dC'_{123}/dP	2.0584741
C_{1112}	8.0187951	dC'_{144}/dP	-1.7668426
C_{1166}	5.7124986	dC'_{456}/dP	1.6209
C_{1122}	8.0187951		
C_{1266}	7.3894107		
C_{4444}	7.9006065		
C_{1123}	-1.9385487		
C_{1144}	-1.9617631		
C_{1244}	-2.3770565		
C_{1456}	-2.0868092		
C_{4466}	-2.35435		

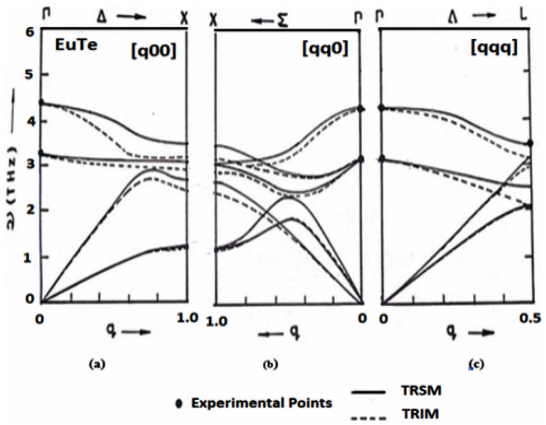

Fig. 1. Phonon Dispersion Curve for [EuTe]

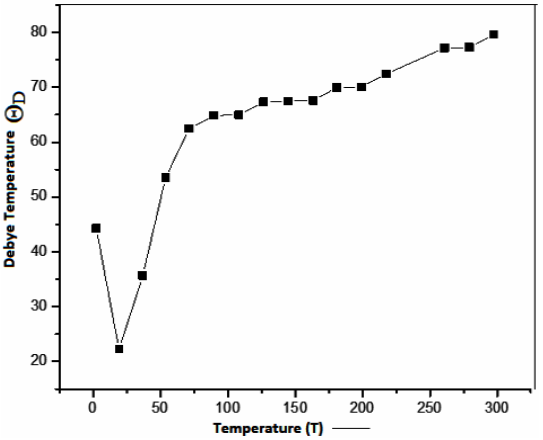

Fig. 2. Debye temperature curve for [EuTe]

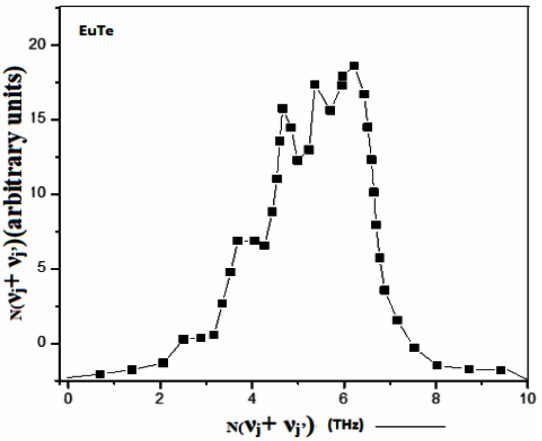

Fig. 3. Combined density of states curve for [EuTe]

RESULTS

The present approach is effectively described the crystal dynamics of (EuTe), eight parameter's with elastic constants (C_{11}, C_{12} & C_{44}), six short range force constants parameters r_0 f_0', ionic charge z, shell charge Y, polarizabilities (α_1, α_2) & polarizability (mechanical) 'd' developed by[16] for (EuTe) are reported in Table 1 by using Eq.1 & 2. The knowledge of lattice vibration frequency (CDSc) reports in Table 2 by computing N (v_j + v'_j) of the combined frequencies (v_j +v'_j). The combined density data is reported in Table 3. The sensitivity of two-phonon Raman spectra is towards high-frequency side of the phonon spectra & specific heats towards its lower side is confirmed the validity of present model for its full wavelength range. The 3rd & 4th order elastic constant and its pressure derivatives for (EuTe) are given in Table 4. Which is probably the first reports in the

absence of experimental data, but their reliability test is not possible. The reported result by use of SNTRSM for (EuTe) is comparatively nearer to the measure data on PDCs, which are showing in the Fig. 1(a), (b) & (c). These results for TMC and its some features of PDC for (EuTe) are specially reporting here. The interactions of three body have affected both LO & TO branches, more than acoustic branches (LA and TA). Other striking feature is excellent reproduction of optical and acoustic branch. The model parameter of TRSM & TRIM is used to calculate the frequency along with uniformity and curve is plotted between wave vectors versus obtain (PD) from this model. These curves are measure up with use of inelastic neutron scattering technique. The specific heat data has been enumerating at variable temperature by Blackmann's[17] and the Debye temperature curve is plotted with absolute temperature (T). Qualitatively the TRSM model is prominent than some of the model values. In addition, some other researchers[18-22] of the same field of research have also tried to report their best to explain PDCs and other properties of europium chalcogenides but only with moderate success. To increase the merit of this work we have calculated 33 two phonon IR/Raman spectra and alteration of Debye temperatures shown in Fig. 2. The (CDS) peaks is compare with theoretical data, shown in Fig. 3. The interpretation of critical point study has been used by Burstein *et al.,*[23]

CONCLUSION

Although, quantitively the agreement achieved from our present model TRSM is good. Furthermore, slight discrepancies still occurring between theory and experiment may be further improved by including the effect of free carrier screening (FCS), Van der Waals interactions (if data are available in future) and by including anharmonic vibrations in the present model (TRSM). A large group of researchers also have successfully reported theoretical results for some other alkali halides and semiconducting materials[24-31] by use of the present model which shows the validity of this model.

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Conflict of interest
Funding facility is not given by any agencies.

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